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<b>13. ABSTRACT (Maximum 200 words)</b>  The work on the behavior of a series of organophosphorus and organoarsenic compounds in superheated water was completed. Additional work was carried out in the area of aquathermolysis of aliphatic, aromatic, and heterocyclic amino compounds and heteroaromatic nitrogen-containing compounds. The results obtained show potential for the detoxication of military wastes by high-temperature supercritical hydrolysis. The work on the property and activity relationships with structures (QSPR/QSAR) was carried out using our recently developed CODESSA (Comprehensive Descriptors for Statistical and Structural Analysis) program containing around 1000 descriptors all of which are calculated only from the molecular structure without requiring any experimental data. We applied this approach for developing models for toxicities, vapor pressures, aqueous solubilities, water-air partition coefficients, critical temperatures, organic solvent scales, glass transition temperatures of polymers, refractive index values for polymers and organic compounds, and other properties. The correlation equations obtained can be successfully used to predict all these physicochemical properties.				
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# **Detoxification of Military Wastes by Nearcritical and Supercritical Water and QSPR Investigations**

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**September 10, 1998**

**U. S. ARMY RESEARCH OFFICE**

**DAAH04-95-1-0497**

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## 1. STATEMENT OF THE PROBLEM STUDIED

During the first plan of the investigation we studied the behavior of representative model compounds in water at high temperatures. The objective was then changed to develop QSPR models for physical, chemical and biological properties of organic compounds.

## 2. SUMMARY OF THE MOST IMPORTANT RESULTS

2.1 The behavior of a series of organophosphorus and organoarsenic compounds in superheated water was studied followed by GC/MS identification of the reaction products. The results demonstrated the ready conversion of two sets of model substrates to lower molecular-weight compounds in aqueous media: (i) phenolic, other substituted aryl, and volatile alkyl/alkenyl organophosphorus compounds; (ii) aryls, haloaralkyl, aryldialkyl, and amino-substituted organoarsenic compounds. Two papers on this work were published in *Toxicological and Environmental Chemistry*. (See 3.1a and 3.1b)

2.2 Additional work in the area of aquathermolysis was carried out on the behavior of aliphatic, aromatic, and heterocyclic amino compounds and heteroaromatic nitrogen-containing compounds. The results further extend the available science base for the behavior of organic compounds on treatment with sub- and super-critical water. The paper has been submitted to (See 3.2)

2.3 The Ames test was studied to measure Mutagenicity, which is one of the properties tested for risk assessment of chemicals. Basing on the values, we developed a QSPR model to predict mutagenicity. The paper has been submitted to *Quantitative Structure Activity Relationship*. (See 3.3)

2.4 A QSPR model on the glass transition temperatures of polymers has been developed and published in the *Journal of Chemical Information and Computer Science*. (See 3.4)

2.5 We have developed a QSPR model for the prediction of the refractive index for organic compounds. A manuscript describing these results has been accepted by the *Journal of Chemical Information and Computer Science*. (See 3.5)

2.6 We have also developed a QSPR model for the prediction of refractive index for polymers. A manuscript describing these results has been accepted by the *Journal of Chemical Information and Computer Science*. (See 3.6)

- 2.7 We have compiled a large set of 45 individual solvent scales of commonly used solvents, and developed QSPR models for them. A principle component analysis has been done on the 45 scales of 40 solvents. Two manuscripts are attached to this report. (See 3.7a and 3.7b)

### 3. LIST OF ALL PUBLICATIONS (No Technical Reports were prepared)

- 3.1 a Aqueous High-Temperature Chemistry of Arsenic-Containing Compounds in Water at 300°C. (A. R. Katritzky, P. A. Shipkova, M. Qi, D. H. Powell, M. Siskin, H. D. Durst) *Toxicol. Environm. Chem.* **1997**, *59*, 239-249.
- 3.1 b Aqueous High-Temperature Chemistry of Organophosphorus Compounds. (A. R. Katritzky, J. V. Pervova, P. A. Shipkova, S. M. Allin, M. Siskin, D. T. Ferrughelli, H. D. Durst) *Toxicol. Environm. Chem.* **1997**, *59*, 219-238.
- 3.2 Reaction of Some Saturated Heterocycles and Related Amines with 49% Formic Acid at 350°C. 27[1]. (A. R. Katritzky, D. A. Nichols, P. A. Shipkova, M. Siskin) *ACH-Models in Chem.* Submitted.
- 3.3 A Comprehensive QSAR Treatment of the Genotoxicity of Heteroaromatic and Aromatic Amines. (U. Maran, A. R. Katritzky, M. Karelson) *QSAR* Submitted.
- 3.4 Quantitative Structure-Property (QSPR) Correlation of Glass Transition Temperatures of High Molecular Weight Polymers. (A. R. Katritzky, S. Sild, V. S. Lobanov, M. Karelson) *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 300-304.
- 3.5 A General QSPR Treatment of the Refractive Index of Organic Compounds. (A. R. Katritzky, S. Sild, M. Karelson) *J. Chem. Inf. Comput. Sci.* Accepted.
- 3.6 Correlation and Prediction of the Refractive Indices of Polymers by QSPR. (A. R. Katritzky, S. Sild, M. Karelson) *J. Chem. Inf. Comput. Sci.* Accepted.
- 3.7 a QSPR Treatment of Solvent Scales. (A. R. Katritzky, T. Tamm, Y. Wang, S. Sild, M. Karelson) Prepared to be submitted to *J. Chem. Inf. Comput. Sci.*
- 3.7 b A Unified Treatment of Solvent Properties. (A. R. Katritzky, T. Tamm, Y. Wang, M. Karelson) Prepared to be submitted to *J. Chem. Inf. Comput. Sci.*

### 4. LIST OF ALL PARTICIPATING SCIENTIFIC PERSONNEL

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